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DESCRIPTION OF THE COMPUTER PROGRAM

Appendix F

of

Development of a Simulation Model
for Estimating Ground Level Concentrations
of Photochemical Pollutants

Prepared by

Systems Applications, Inc.
Beverly Hills, California 90212

for the

Air Pollution Control Office
of the Environmental Protection Agency
Durham, North Carolina 27701

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Emphasis was placed on the preparation of an efficient program and on insuring the applicability of the program in any urban airshed. An airshed is essentially defined by its terrain, meteorological, and source inputs. Since these parameters are all treated as input data to the program, no difficulty should be encountered in applying the program in a variety of urban airsheds. The most cumbersome aspect of program usage is the large effort required in the preparation of the meteorological input data. Two programs are used in the Los Angeles Basin simulation effort. The main program, the Atmospheric Pollution Simulation Program, calculates pollutant concentrations as a function of space and time using source and meteorological inputs. The structural and the operational aspects of this program are discussed. Aircraft emissions are treated as input to this program via magnetic tape. The computer program which generates this tape, The Aircraft Emissions Program, is also discussed.

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INTRODUCTION

The purpose of this Appendix is to describe in a general way the various facets of the computer program that comprise the urban airshed model. The development of this program is an involved undertaking, as a wide variety of calculations are required both in the numerical solution of the governing equations and in the handling and manipulation of source and meteorological data. Emphasis was placed on the preparation of an efficient program and on insuring the applicability of the program in any urban airshed.

Computational efficiency is vital in two respects. First, it is important to minimize the number of calculations that must be carried out in any large-scale computing effort, particularly when these calculations are a part of iterative loops or are of a repetitive nature. Second, the numerical solution of three dimensional, coupled, time dependent partial differential equations is, apart from data input, handling, and processing considerations, a very time consuming calculation, and efficiency is paramount. With regard to the general applicability of the program, an airshed is essentially defined by its terrain, meteorological, and source inputs. Since these parameters are all treated as input data to the program, no difficulty should be enccountered in applying the program in a variety of urban airsheds.

At this time, the most cumbersome aspect of program usage is the large effort required in the preparation of the meteorological input data (see Appendix C). Incorporation of an interpolation scheme into the program which automatically constructs wind and inversion maps from the raw monitoring station data would alleviate this difficulty. Such an addition to the existing program is required prior to the validation of the model for a large number of different meteorological conditions. It is also worthwhile to remind the reader that, in general, a sizable effort is needed for the preparation of the source emissions inventory for any large urban area. However, it should be noted that, while the spatial and temporal distributions of pollutant emissions are generally the same from day to day (with the exception of the weekend), the meteorology is likely to undergo daily variations. Thus, the emissions inventory must be undertaken only once. If the model is to be used in testing control strategies, it will become necessary to alter the source input data. Such alterations should present few difficulties, however, from the standpoint of program operation.

Two programs are ~~currently being~~ used in the Los Angeles Basin simulation effort. The main program, the Atmospheric Pollution Simulation Program, calculates pollutant concentrations as a function of space and time using source and meteorological inputs. ~~We discuss both~~ the structural and the operational aspects of this program, ~~in Section I of this Appendix.~~ Aircraft emissions are treated as input to this program via magnetic tape. The computer program which generates this tape, The Aircraft Emissions Program, is discussed in Section II.

I. THE ATMOSPHERIC POLLUTION SIMULATION PROGRAM

The Atmospheric Pollution Simulation Program accepts source and meteorological data as inputs to produce pollutant concentration/time histories at discrete points distributed throughout the airshed. The code consists of a MAIN program and several subroutines which perform specialized tasks. In its present configuration, the program utilizes two magnetic tape units and temporary disc storage. Currently, the program size is approximately 350K bytes.

Inputs to the program are contained on cards and two magnetic tapes. The following information is supplied via punched cards:

- the horizontal extent and topography of the airshed
- the time span over which the simulation is to take place
- the spatial and temporal grid size
- the time interval for concentration printout
- the chemical species to be simulated
- the maximum number of iterations allowed in Step I of the numerical solution of the governing equations
- freeway and non-freeway vehicle mileage distributions
- fixed source emissions
- the chemical reaction rate constants
- the initial concentration distribution

The two magnetic tapes mentioned above contain meteorological and aircraft emissions data respectively. The meteorological data consists of wind speed and direction, mixing depth, and temperature for each column of grid points. Each set of data is applicable for a certain time interval (say, between 0630 and 0730 PST), and this time interval is recorded on the tape immediately preceding each set of data. Before a simulation begins, the program reads the tape until it locates a set of data applicable at the starting time of the simulation. Similarly, the aircraft emissions tape contains sets of data preceded by a time interval. This tape is also automatically positioned before the simulation begins. The aircraft emissions tape is generated by the Aircraft Emissions Program, discussed in Section II, and consists of pollutant emissions rates (ppm/minute) into each cell of the airshed.

The primary output of the program is a printout of the hourly-averaged ground-level concentration distribution for each chemical species simulated. These concentration maps, in standardized output format, can be easily compared with observed pollutant levels. It should be noted, however, that the number of concentration values that are computed is generally quite large. Thus, we do not attempt to display the entire concentration field at any time. It is felt that generally the ground-level concentrations will be of most interest since measurements of pollutant levels aloft are scarce. With this in mind, we have included an output option which allows the user to monitor the progress of the simulation with an appropriate level of detail. The program prints the instantaneous

ground-level concentrations and user-selected vertical concentration profiles at regular time intervals. The user chooses ground-level coordinates of points of interest, and the program prints all concentrations between the ground and inversion base at those points. In simulations performed thus far, we have sampled the instantaneous concentrations every twenty minutes and have chosen to examine the vertical concentration profiles only above monitoring stations. We have found this display of output to be quite satisfactory for this phase of model development.

In future phases of program development, we plan to investigate alternative means of presenting the results of a simulation. Such a presentation will probably include the use of graphical techniques to display ground-level concentration contour maps and vertical concentration profiles. Moreover, the present treatment of data input to the program is by no means final, and, in fact, only represents a convenient means for satisfying current needs. When the model is completed, treatment of input will be re-evaluated. At that time we will be able to make recommendations as to how the input should be handled. A foreseeable change in the input structure will occur, for example, if we develop an interpolation scheme to construct the wind field directly from the monitoring station data.

The remainder of this discussion will be segmented into two parts. In Section A we describe the overall structure of the program and discuss the role played by each subroutine subprogram. Section B is devoted to a generalized, step-by-step description of how the program operates during a typical simulation run.

A. The Structure of the Atmospheric Pollution Simulation Program

In this section we describe the various subprograms that comprise the main program, giving details of how they operate and referring to appropriate portions of the main text and appendices for detailed discussions of the underlying concepts involved. In Figure F-1 we indicate schematically the overall structure of the program, and in Table F-1 we list each subprogram and summarize its function.

MAIN

MAIN is responsible for two aspects of a simulation:

(1) the control of model initialization
(2) the numerical integration of the governing airshed equations

Model initialization consists of defining the physical characteristics of the airshed (horizontal extent and topography), reading source emissions data, positioning data tapes, establishing the grid on which

Figure F-1 and Table F-1 follow

FIGURE F-1. STRUCTURE OF THE ATMOSPHERIC POLLUTION SIMULATION PROGRAM

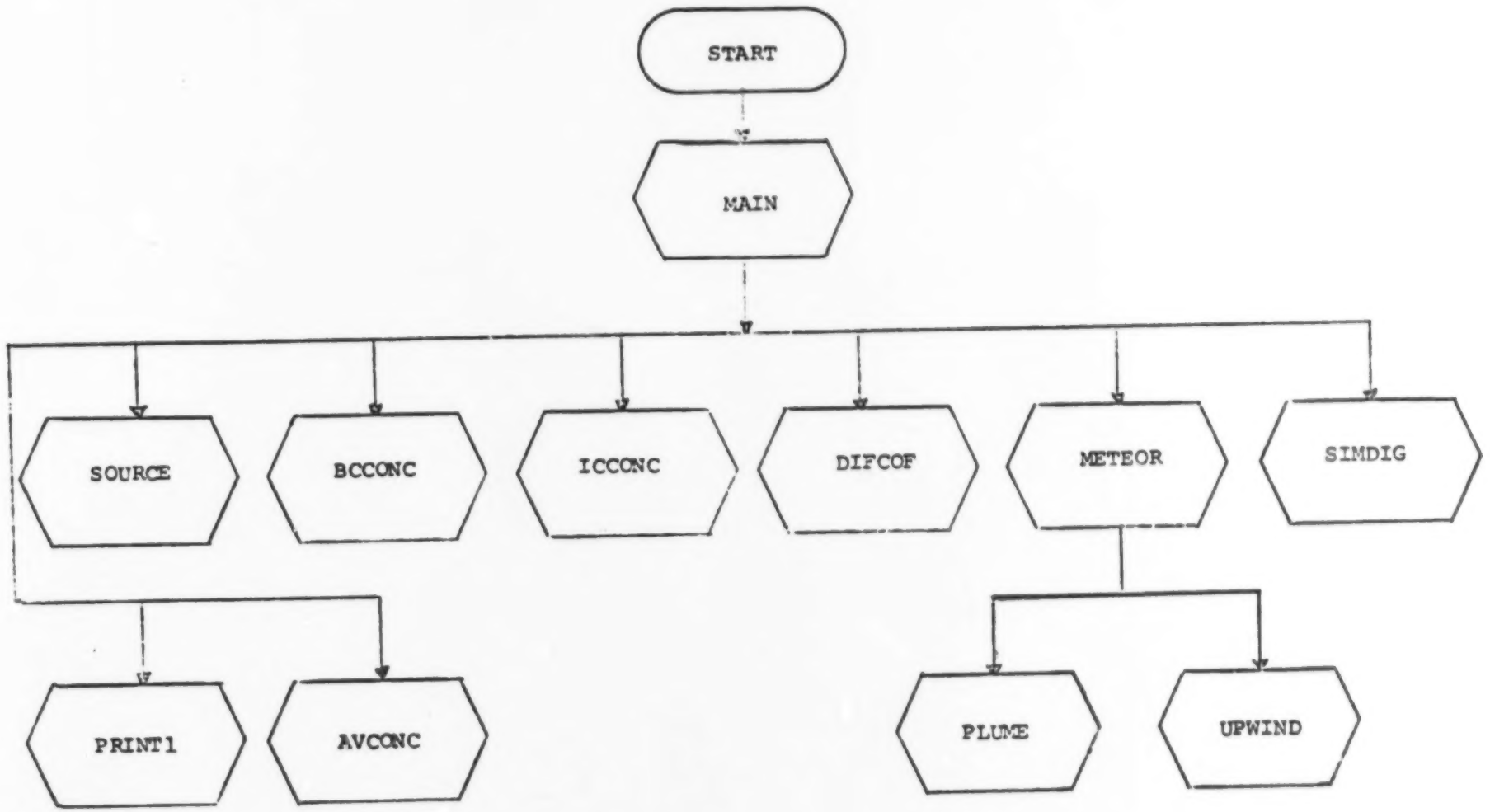


TABLE F-1. SUMMARY OF SUBPROGRAMS AND THEIR FUNCTION

ROUTINE	FUNCTION
MAIN	initialization of the model and the numerical solution of the governing airshed equations
AVCONC	calculates and prints hourly-averaged ground level pollutant concentration maps
BCCONC	supplies boundary concentrations at points of horizontal inflow into the model
DIFCOF	calculates the turbulent eddy diffusivity at each point in a given column of grid points
ICCONC	sets up the initial concentration distribution
METEOR	reads lower wind field and inversion base elevations and alters the vertical concentration distribution due to temporal changes in the inversion base elevations
PLUME	calculates the spatial distribution of power plant emissions
PRINT1	prints instantaneous ground-level pollutant concentration maps as wellas user-selected vertical concentration profiles
SIMDIG	solves system of linear equations whose coefficient matrix is tridiagonal
SOURCE	calculates automotive and fixed source pollutant emissions (except power plants)
UPWIND	calculates the upper wind field

the numerical integration is to take place, and entering the initial concentration distribution. However, not all of these functions take place in MAIN. The sequencing involved in model initialization is described in more detail in Section B. When model initialization is complete, the numerical integration procedure may be initiated.

Before an integration time step can be taken, source and meteorological variables must be updated. Subroutines SOURCE, METEOR, and PLUME are called to supply vehicular and fixed source emissions, meteorological data, and power plant emissions respectively. Also, aircraft emissions are obtained from the temporary disc area, and subroutine DIFCOF is called to supply values of the eddy diffusivity. The numerical integration now proceeds with the sequential solution of Steps I, II, and III as described in Appendix D.

When the simulation is complete, the program punches the final concentration distribution onto cards. This enables the user to restart the integration at a later date. In early stages of model validation, we have found it convenient to divide a 12-hour simulation into three four-hour model runs, thereby allowing us to monitor the progress of the simulation. If, after a four-hour segment, the predicted concentrations are found to be acceptable, we merely use the punched concentrations as initial conditions to continue the simulation further in time.

AVCONC

Subroutine AVCONC is called from MAIN after every integration time step and is responsible for the calculation and printout of hourly-averaged ground level concentration maps. Each time AVCONC is entered, an array is incremented by the current values of the ground level concentrations. After one hour, this array is divided by the number of time steps taken over that hour so as to produce an array of hourly-averaged pollutant levels. By manually superposing the actual monitoring station observations on these maps, one can easily evaluate the model's performance.

BCCONC

Subroutine BCCONC supplies pollutant levels at points on the airshed boundary where horizontal inflow takes place. Generally, the actual concentrations are not known, and hence the values used are merely educated guesses. If levels were known, then they could be input on cards or tape. In current simulation efforts involving CO, we have employed boundary concentrations of 3 ppm at all points of horizontal inflow.

DIFCOF

In Step I of the numerical integration and during the cubic spline interpolation procedure, it is necessary to have values of the turbulent eddy diffusivity. Subroutine DIFCOF supplies values of the diffusivity

for a vertical column of grid points. The coordinates of the column are transferred to DIFCOF, and diffusivities are calculated from knowledge of the meteorological conditions in the column (see Appendix C for a discussion of the algorithm employed).

ICCONC

The initial concentration distribution is established through subroutine ICCONC. This subroutine assumes two forms, depending on the mode of initial concentration input. In the first mode, the initial ground-level concentrations are read from cards which were prepared from ground-level concentration maps that are based on actual observed pollutant levels. The values in the ground cells are extended vertically to the inversion to complete the definition of the initial concentration field. The second mode of input arises when a simulation begins at a point in time at which a previous simulation terminated. As was mentioned in the discussion of the MAIN program, at the end of a simulation the entire concentration field is punched onto cards. Thus the second mode simply consists of a READ statement to read the punched cards.

METEOR

The processing of the meteorological data is the domain of subroutine METEOR. During model initialization, METEOR is called by MAIN, and the meteorological input tape is read until data applicable at the start of the simulation are encountered. As the simulation progresses, the meteorological variables are updated as necessary by reading the tape. See Appendix C for a further discussion of the meteorological data. When inversion elevations change, it becomes necessary to transfer the concentration field from the old grid to the new grid. A cubic spline procedure is employed which requires values of the diffusivity as supplied by DIFCOF. A system of linear equations must be solved, and subroutine SIMDIG performs this task. Finally, subroutines UPWIND and PLUME are called to supply the upper wind field and the spatial distribution of power plant emissions, respectively.

PLUME

Subroutine PLUME computes the spatial and temporal distribution of power plant emissions. Since the spatial distribution varies with changes in meteorological variables (every hour in this case), it was convenient to call this subroutine from METEOR. A detailed discussion of the method used to distribute the power plant emissions may be found in Section III of Appendix A.

PRINT1

The results of the numerical integration are printed in subroutine PRINT1. User-selected vertical concentration profiles and ground-level

concentration maps are printed at regular time intervals. We have found that an interval of 20 minutes between printouts gives a good indication of hourly trends and does not result in endless pages of unused computer output. Predicted vertical concentration profiles in the vicinity of monitoring stations are also printed out at the option of the user.

SIMDIG

Subroutine SIMDIG solves a system of linear equations whose coefficient matrix is tridiagonal. Thomas' algorithm is employed in the solution (see von Rosenberg (1969) for details). The three bands of the matrix and the known vector are transferred to the subroutine, and the solution is returned upon completion.

SOURCE

Automotive and fixed source emissions (with the exception of power plant emissions) are computed in subroutine SOURCE. All emissions are treated as surface fluxes. See Appendix A for a complete discussion of the source inventory.

UPWIND

Subroutine UPWIND computes the wind field aloft. When the lower wind field is completely defined in METEOR, control is passed to UPWIND. We refer the reader to Appendix C for a discussion of the algorithm employed.

B. Program Operation

In this section we discuss, in a general manner, the operation of the program during a typical simulation. Since neither the model nor the program have taken final form, a complete card-by-card description would be lengthy and of no particular value at this juncture. Figure F-2 should be referred to throughout this discussion, as a schematic representation of the order of the computational operations is shown therein.

A simulation commences in MAIN with the input of all information contained on punched cards, with the exception of the initial concentration distribution, which is input later. The program then reads the aircraft emissions tape until it encounters data applicable at the time the simulation is to start. At this point the program calculates all the parameters that will be used in the numerical integration of the governing airshed equations. For example, partial derivatives of the terrain elevation

$$\frac{\partial h}{\partial x} \quad \text{and} \quad \frac{\partial h}{\partial y}$$

where $h(x,y)$ = terrain elevation at x,y

are approximated by finite differences. After all necessary parameters are calculated, subroutine METEOR is called to position the meteorological data tape. As before, this is accomplished by reading the tape until data applicable at the start of the simulation is encountered. Control then passes to subroutine ICCONC where the initial concentration field is established. Finally, subroutine SOURCE is entered, and the automotive and fixed source emissions distributions are initialized for future use. Model initialization is now complete, and PRINT1 is called to print the initial concentration distribution.

The MAIN program now enters the "computational loop," in which the governing partial differential equations are integrated numerically. Each pass through this loop results in advancing the simulation time by the value of one time step (1 to 5 minutes). Before a forward step in time can be made, however, photochemical, meteorological, and source variables must be updated. First, chemical reaction rate constants are calculated. (See Section VI-A in Appendix B for a discussion of the temporal variation of the photolysis rate constants.) Next, subroutine METEOR is called to update the meteorological variables. If the currently stored data are applicable at the time of the call, then control immediately returns to MAIN. Recall that the meteorological variables are held constant for a period of one hour. If the data are no longer current, then the meteorological data tape is read, and new values of the meteorological variables are calculated. Upon return from METEOR, subroutine SOURCE is entered, and new values of the automotive and fixed source emissions are computed. If the aircraft emissions rates stored in the temporary disc area are no longer applicable, then the next set of emissions is transferred from the tape to the disc area. This completes the definition of the photochemical, meteorological, and source variables. We are now ready to proceed with the numerical integration of the governing airshed equations.

The numerical integration takes place in three sequential steps. In Step I we move from column to column solving the ρ-direction convection-diffusion equation. The procedure followed in the solution of one column of points (or nodes) will be described. Power plant and aircraft emissions into the column are established first. The turbulent eddy diffusivity at each point in the column is then calculated in DIFCOF. Since Step I involves the iterative solution of implicit difference equations, the computation primarily involves solving systems of linear equations of the form

$$Ax = y$$

where A = tridiagonal matrix
x = solution vector
y = known vector

We thus compute A and y, and then call SIMDIC which returns x. Each component of the solution vector represents the concentration at one point in the column. When the iteration has converged at a given column, we repeat the calculation for the next column. Step I is complete when these computations have been carried out for all columns.

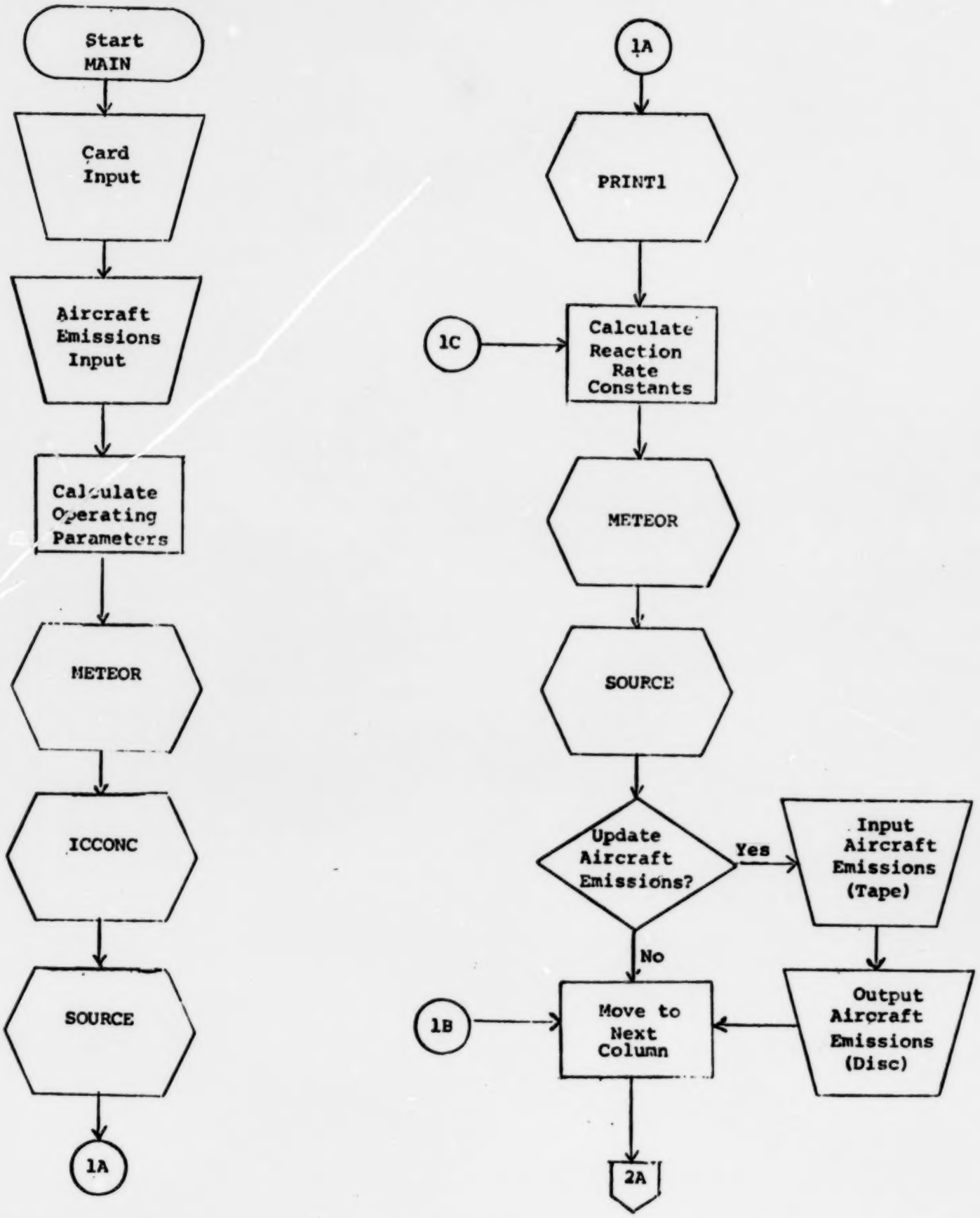
Before Step II can be initiated, subroutine BCCONC must be called to provide pollutant concentration levels at points of horizontal inflow on east and west boundaries. Upon return from BCCONC, Step II proceeds as described in Appendix D. When Step II is complete, BCCONC is again called, but this time to supply concentration levels for the north and south boundaries. The computation of Step III then follows. At the conclusion of Step III, the numerical integration procedure is completed for a single time step.

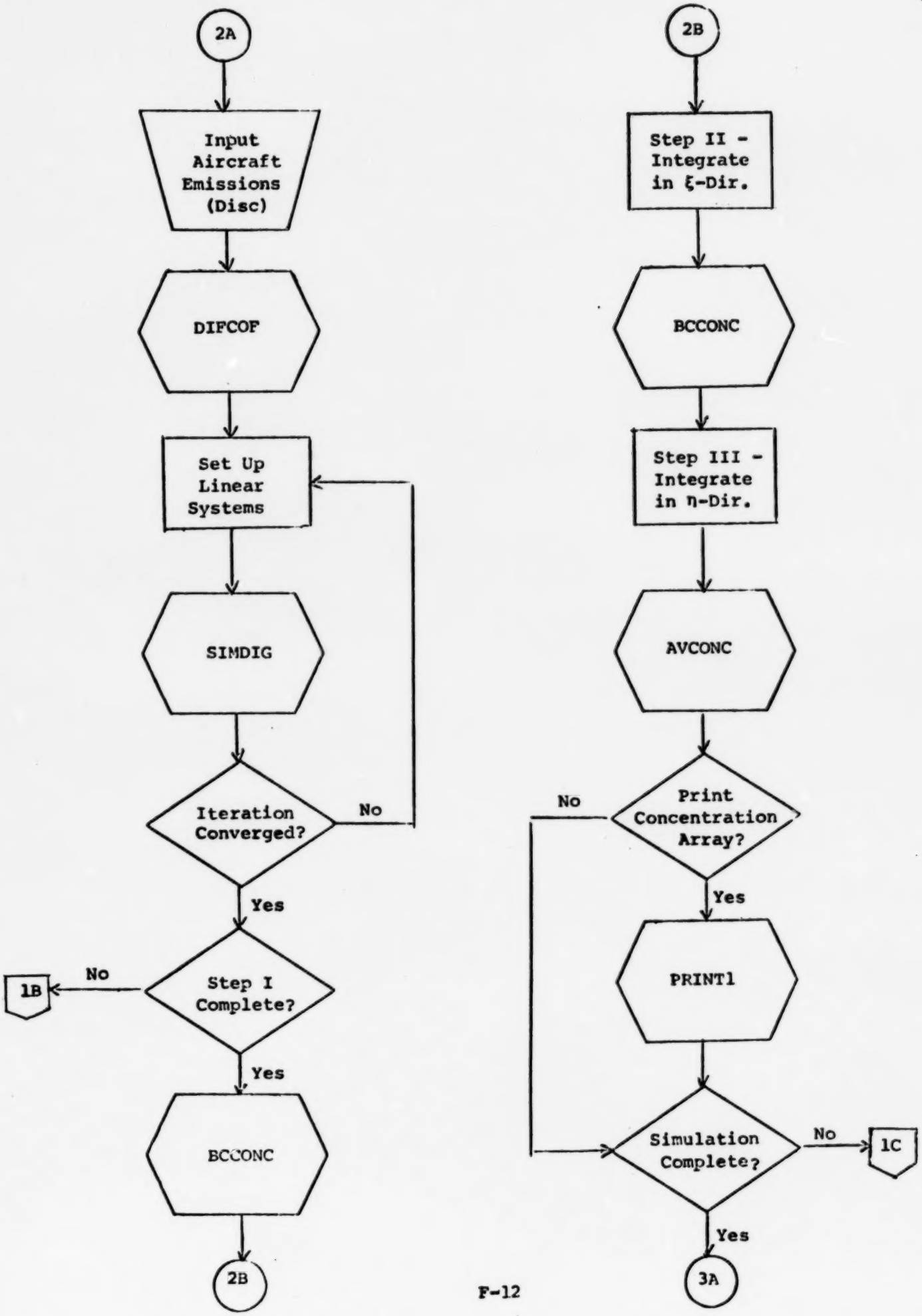
Subroutine AVCONC is now entered, and the hourly-averaged ground-level concentration array is incremented by the new ground-level concentrations. If an hour has elapsed, then the array is divided by the number of time steps taken over that hour. AVCONC then proceeds to print an average concentration map for each chemical species.

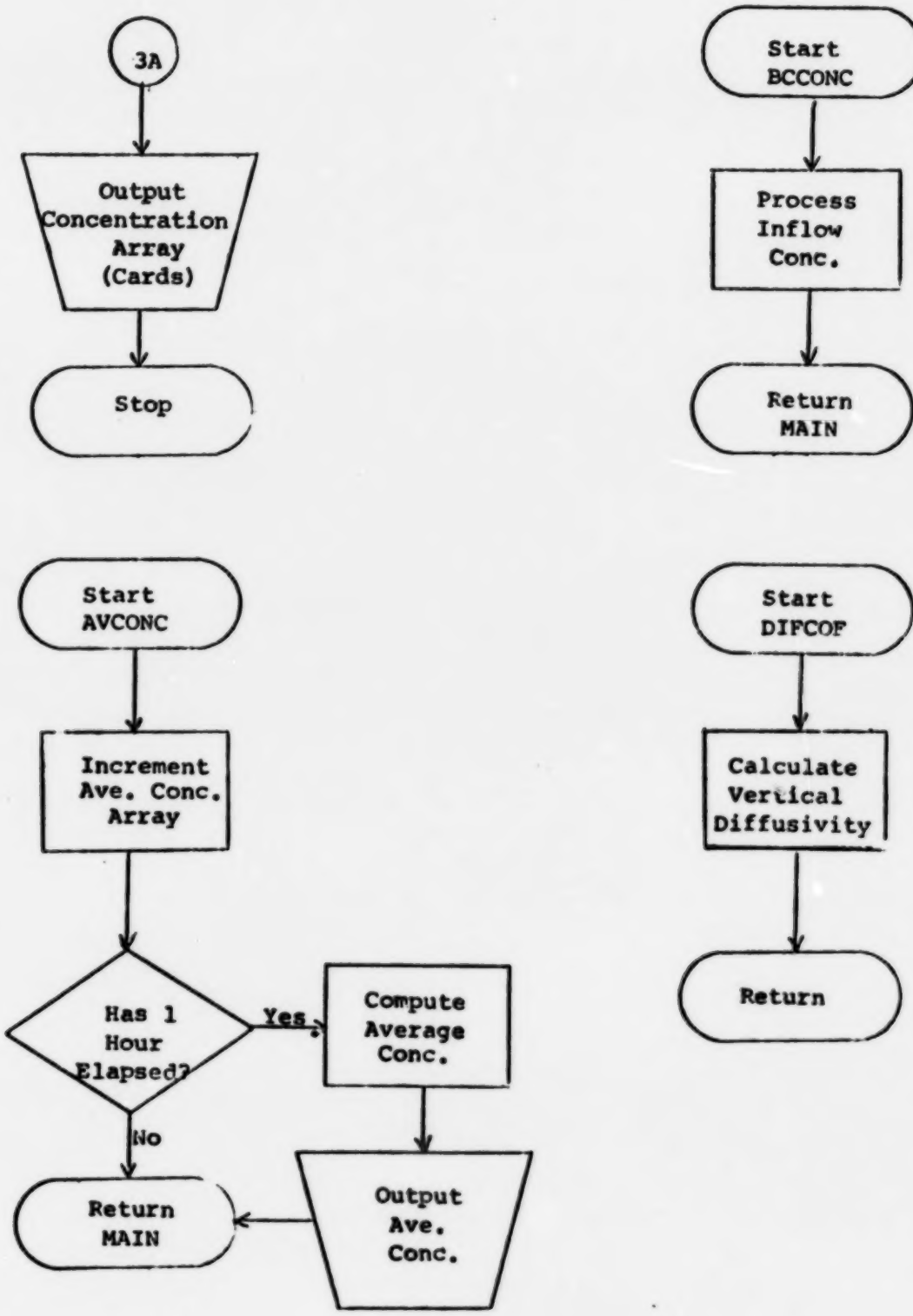
Instantaneous ground-level concentration maps and user-selected vertical concentration profiles are printed at regular time intervals (say, every 20 minutes). The program checks to see if PRINT1 should be called to perform the output task.

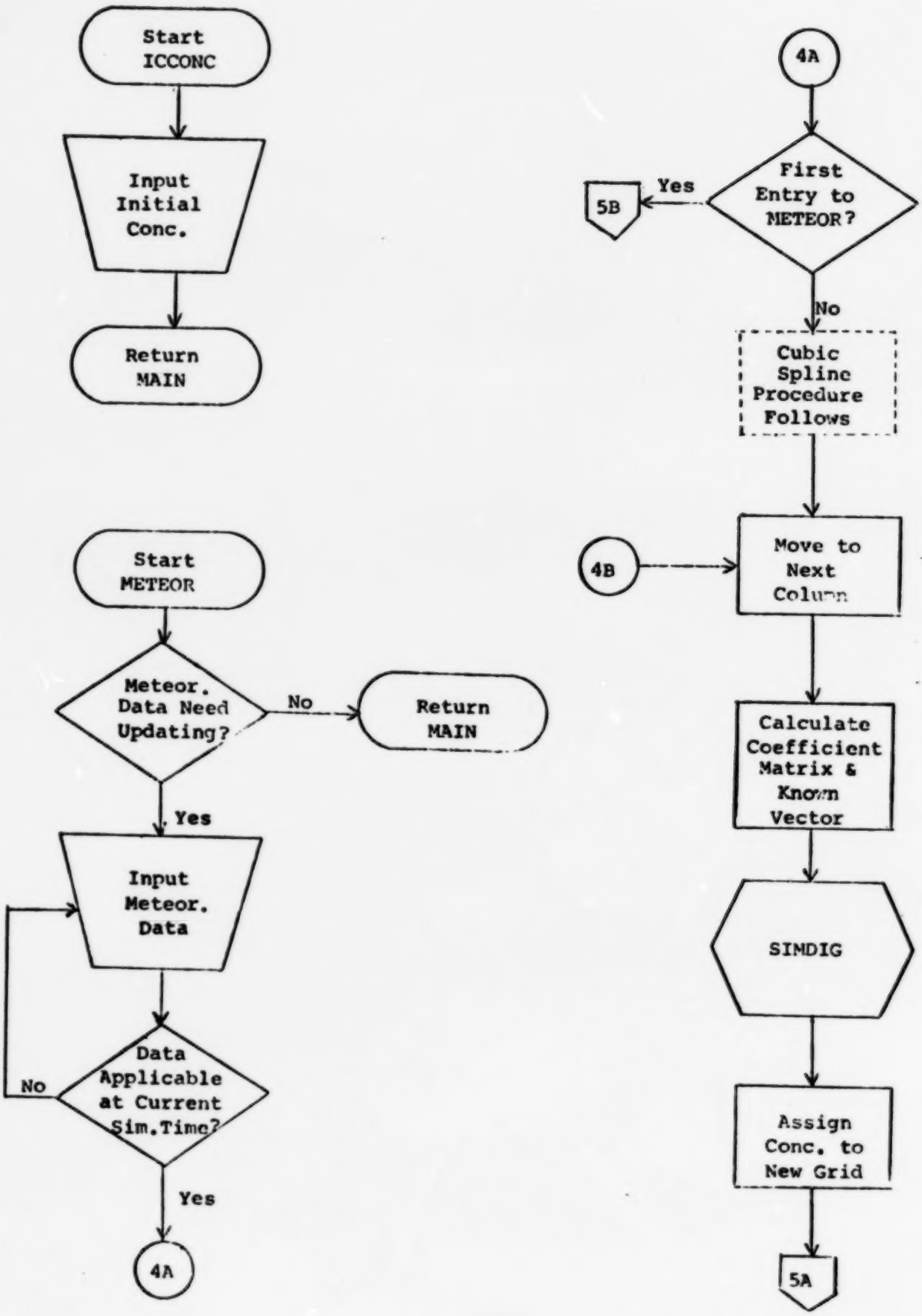
We have now made one complete pass through the "computational loop." If the simulation is to be continued, then control passes to the beginning of the "loop," and the process described above is repeated. When the simulation is terminated, the entire concentration field is punched onto cards. This enables the user to re-start a simulation at some later time.

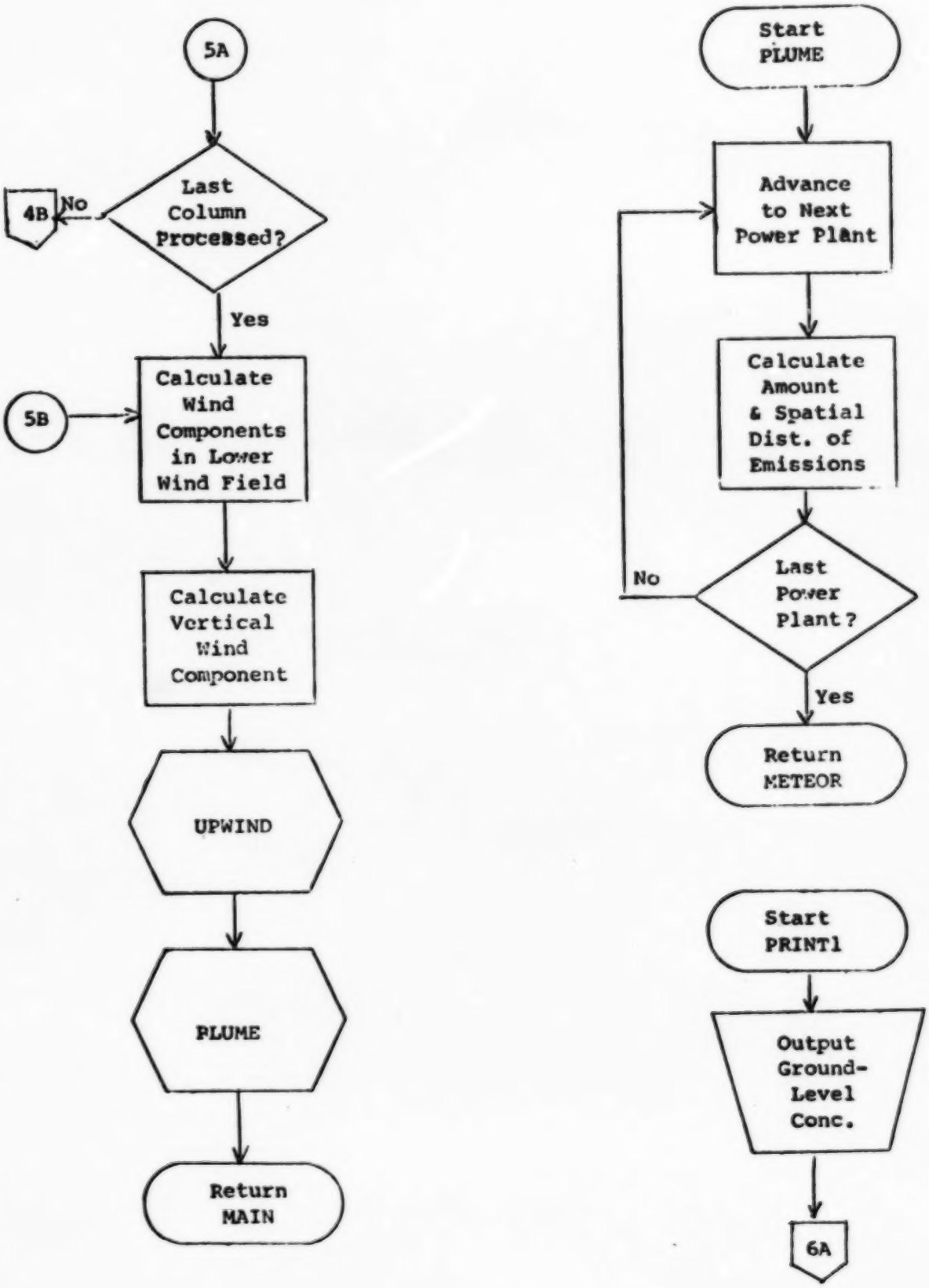
FIGURE F-2. FLOW DIAGRAM OF THE ATMOSPHERIC POLLUTION SIMULATION PROGRAM

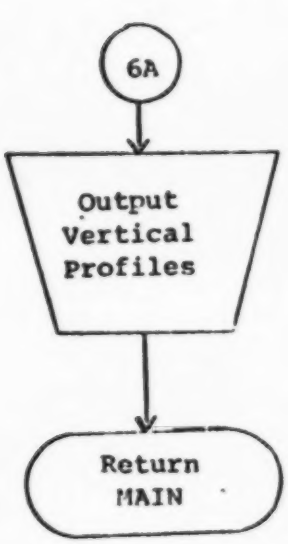


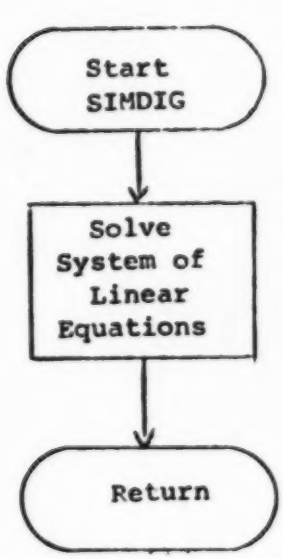

2A
Input Aircraft Emissions (Disc)
DIFCOF
Set Up Linear Systems
SIMDIG
Iteration Converged?
No
Yes
Step I Complete?
No
1B
Yes
BCCONC
2B
2B
Step II - Integrate in ξ-Dir.
BCCONC
Step III - Integrate in η-Dir.
AVCONC
Print Concentration Array?
No
Yes
PRINT1
Simulation Complete?
No
1C
Yes
3A

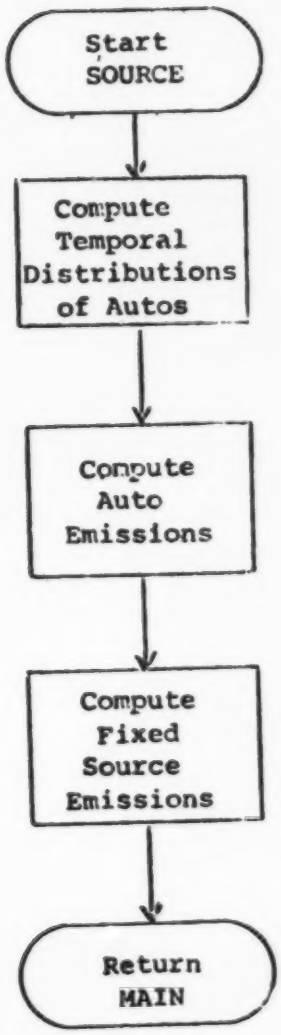

3A
Output Concentration Array (Cards)
Stop
Start BCCONC
Process Inflow Conc.
Return MAIN
Start AVCONC
Increment Ave. Conc. Array
Has 1 Hour Elapsed?
Yes
No
Compute Average Conc.
Output Ave. Conc.
Return MAIN
Start DIFCOF
Calculate Vertical Diffusivity
Return

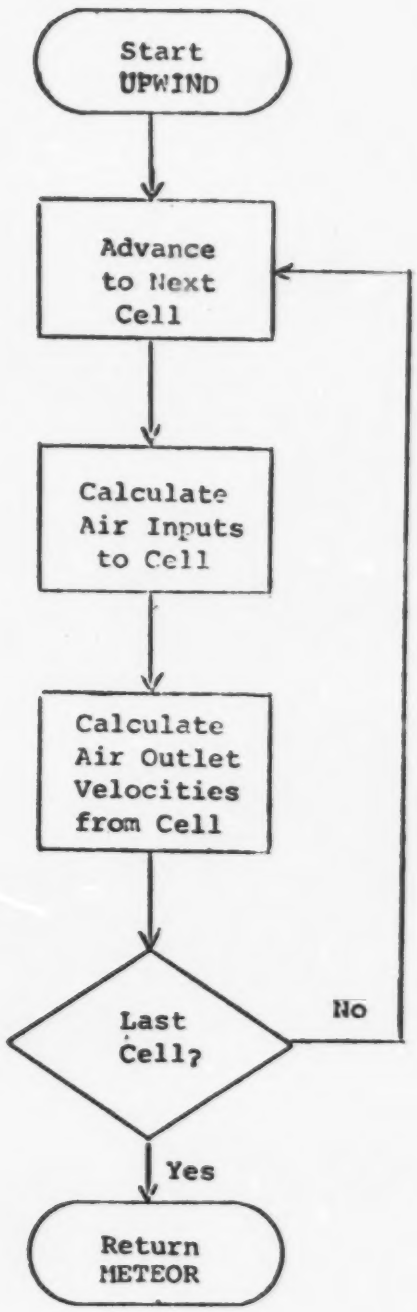

Start ICCONC
Input Initial Conc.
Return MAIN
Start METEOR
Meteor. Data Need Updating?
No
Return MAIN
Yes
Input Meteor. Data
Data Applicable at Current Sim.Time?
No
Yes
4A
4A
First Entry to METEOR?
Yes
5B
No
Cubic Spline Procedure Follows
4B
Move to Next Column
Calculate Coefficient Matrix & Known Vector
SIMDIG
Assign Conc. to New Grid
5A


5A
Last Column Processed?
No
4B
Yes
5B
Calculate Wind Components in Lower Wind Field
Calculate Vertical Wind Component
UPWIND
PLUME
Return MAIN
Start PLUME
Advance to Next Power Plant
Calculate Amount & Spatial Dist. of Emissions
Last Power Plant?
No
Yes
Return METEOR
Start PRINT1
Output Ground-Level Conc.
6A


6A
Output Vertical Profiles
Return MAIN


Start SIMDIG
Solve System of Linear Equations
Return


Start SOURCE
Compute Temporal Distributions of Autos
Compute Auto Emissions
Compute Fixed Source Emissions
Return MAIN


Start
UPWIND
Advance
to Next
Cell
Calculate
Air Inputs
to Cell
Calculate
Air Outlet
Velocities
from Cell
Last
Cell?
No
Yes
Return
METEOR

II. THE AIRCRAFT EMISSIONS PROGRAM

The Atmospheric Pollution Simulation Program, described in Section I, reads aircraft emissions from a magnetic tape created by the Aircraft Emissions Program. The aircraft emissions model consists of two major parts: ground operations and airborne operations. Emissions from these operations are treated as lumped volume sources, generated in the cell into which they are injected. We refer the reader to Section II of Appendix A for a discussion of the governing model.

The Aircraft Emissions Program consists of a MAIN program and a subroutine AIR1. Subroutine AIR1 calculates emissions for both the flight and ground operation modes from aircraft and airport data transferred from MAIN. Input to the program consists of:

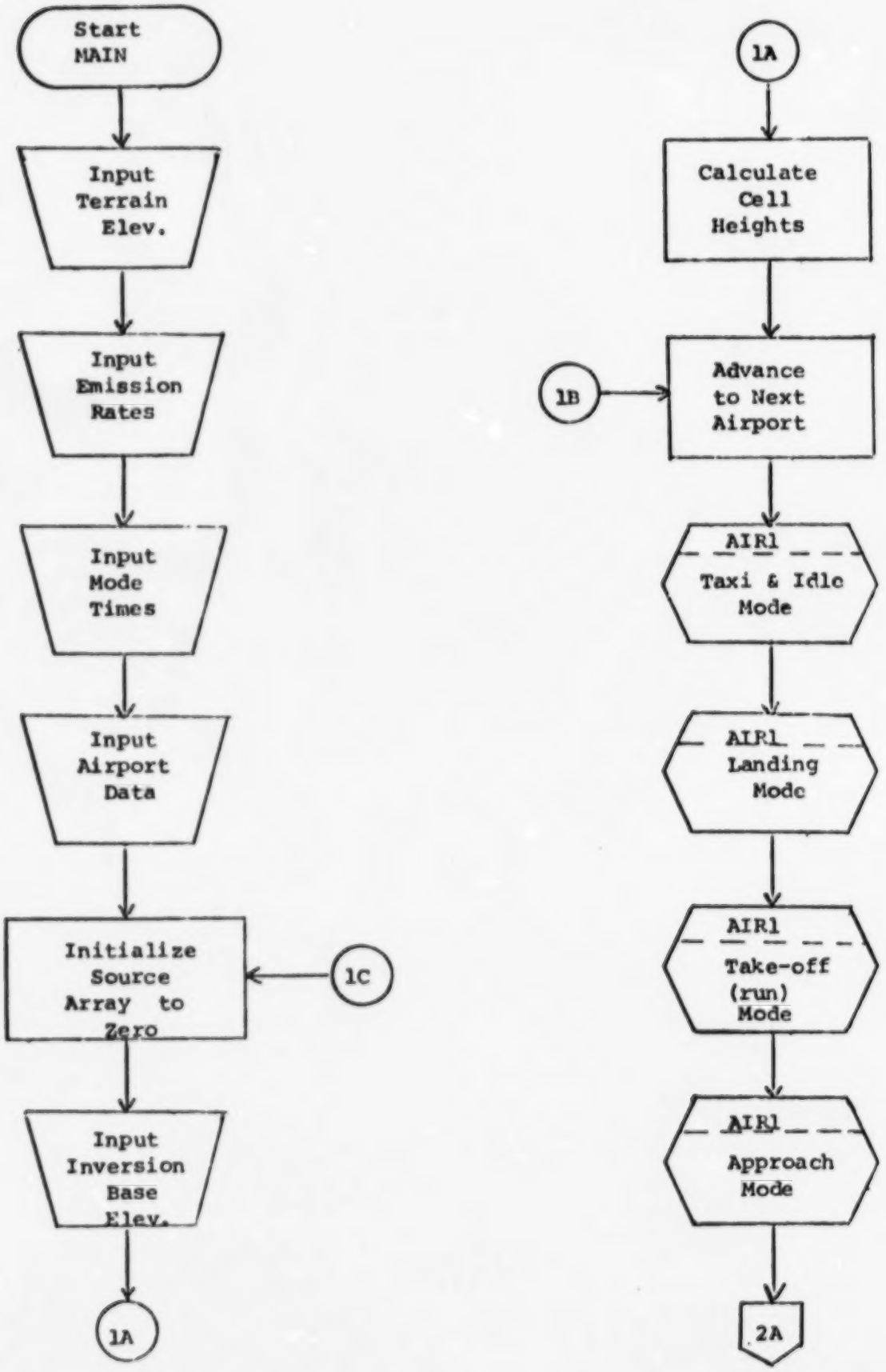
- terrain elevations
- emissions rates tabulated according to aircraft class, operating mode, and chemical species
- the time spent by each class of aircraft in each operating mode
- individual airport data, including location of the airport on the grid and ground and flight operation characteristics
- meteorological data, such as inversion base elevations

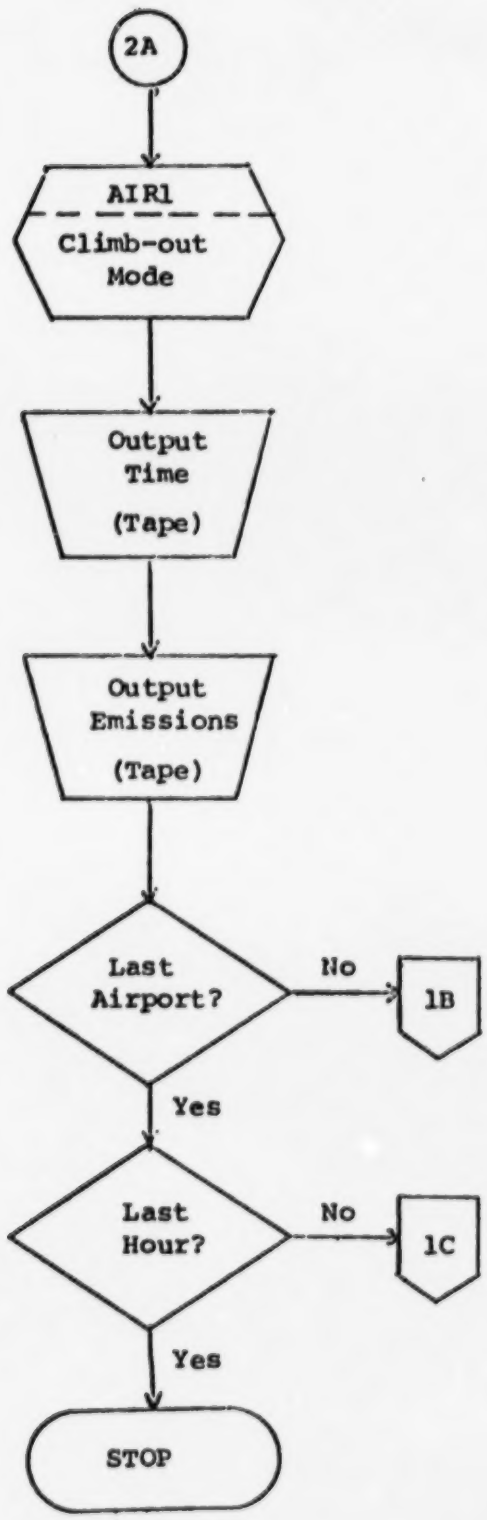
The program uses this information to calculate aircraft emissions into those cells in which airplanes operate. The output of the program, i.e., the pollutant emissions rates into each cell of the airshed, is recorded on the aircraft emissions tape for use by the Atmospheric Pollution Simulation Program.

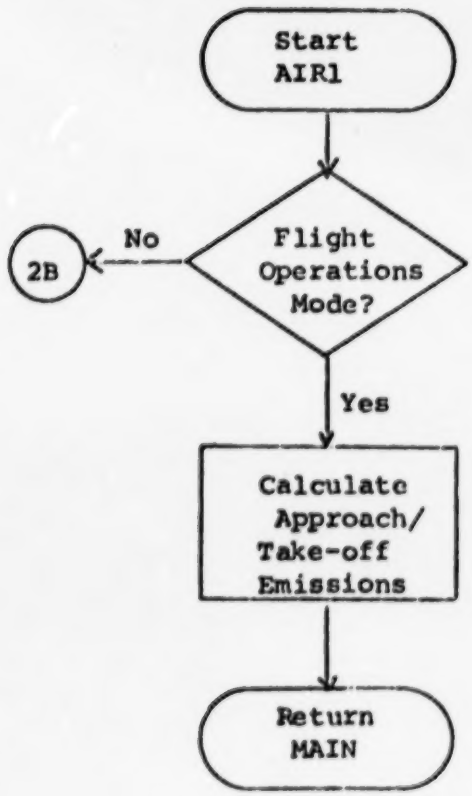
Program operation starts in MAIN with the input of the first four items listed in the preceding paragraph, all of which are contained on punched cards. (See the schematic flow chart in Figure F-3.) We then begin the calculation of the aircraft emissions for each hour or, for that matter, for any other time interval of the simulated day. The emissions into each cell are stored in a large array, which must be initialized to zero. The inversion base elevations are obtained from the meteorological data tape, and cell heights are calculated from (inversion base elevation - terrain elevation)/10, where 10 is equal to the number of horizontal strata. We now calculate the emissions from each airport due to both ground and flight operations. Pertinent information about each mode of operation (e.g., take-off, taxi, landing, etc.) is transferred to AIR1, and the source array is incremented appropriately. After the emissions from each airport have been computed, the time of day and the source values are written on the magnetic tape. If further calculations are to be made, then the source array is again initialized, and the above sequence takes place for another time interval.

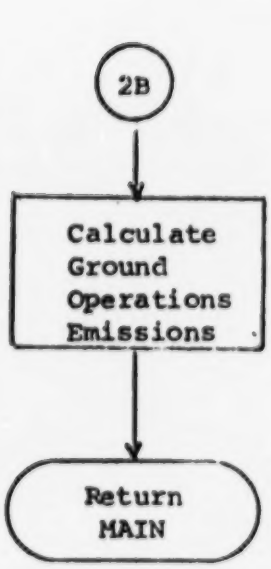
It should be noted that this program can also function as a subroutine in the Atmospheric Pollution Simulation Program. We have operated the aircraft program separately to minimize the storage requirements for the Atmospheric Pollution Simulation Program. In future program development efforts, we will investigate further the question of integrating the Aircraft Emissions Program with the main simulation program.

FIGURE F-3. THE AIRCRAFT EMISSIONS PROGRAM




2A
AIR1
Climb-out Mode
Output Time (Tape)
Output Emissions (Tape)
Last Airport?
No
1B
Yes
Last Hour?
No
1C
Yes
STOP


Start AIR1
Flight Operations Mode?
No
2B
Yes
Calculate Approach/ Take-off Emissions
Return MAIN


2B
Calculate Ground Operations Emissions
Return MAIN

REFERENCES

von Rosenberg, D. U., "Methods for the Numerical Solution of Partial Differential Equations," American Elsevier Publishing Company, New York (1969).